IN THE CLAIMS:

1. (Presently amended) A computer-implemented method for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, ~~comprising executing, via a computer, the following steps:~~ wherein the method is run on a system comprising one or more distinct devices, each of the one or more distinct devices being embodied on a tangible computer-readable recordable storage medium, the method comprising:

calculating a centroid of residue centroids, wherein calculating the centroid of residue centroids is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of calculating the centroid;

using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment, wherein using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of using the centroid as a spatial origin;

calculating a first-order hydrophobic moment, wherein calculating the first-order hydrophobic moment is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of calculating the first-order hydrophobic moment;

enhancing correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric, wherein enhancing correlation between residue centroid magnitude and residue solvent accessibility is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of enhancing correlation;

using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, and wherein each residue centroid having a same fractional distance to a surface of the tertiary protein structure as one or more additional residue centroids contributes an equivalent magnitude

to the global linear hydrophobic moment as the one or more additional residue centroids by mapping each residue at a same distance from a center of the protein structure, wherein using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment;

using the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure, wherein using the global linear hydrophobic moment to characterize the amphiphilicity of the tertiary protein structure is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of using the global linear hydrophobic moment to characterize the amphiphilicity of the tertiary protein structure; and

outputting the global linear hydrophobic moment to a user.

2. (Canceled)

3. (Original) The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.

4. (Original) The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

5. (Original) The method of claim 1, wherein the centroid of residue centroids represents a geometric center of the tertiary protein structure.

6. (Cancelled)

7. (Original) The method of claim 1, wherein the global linear hydrophobic moment characterizes a magnitude of amphiphilicity of the tertiary protein structure.

8. (Original) The method of claim 1, wherein the global linear hydrophobic moment characterizes a direction of amphiphilicity of the tertiary protein structure.

9. (Original) The method of claim 1, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

10. (Cancelled)

11. (Cancelled)

12. (Cancelled)

13. (Cancelled)

14. (Presently amended) An apparatus for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, the apparatus comprising:

a memory; and

at least one processor operative to:

calculate a centroid of residue centroids;

use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

calculate a first-order hydrophobic moment;

enhance correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

use the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global

linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, and wherein each residue centroid having a same fractional distance to a surface of the tertiary protein structure as one or more additional residue centroids contributes an equivalent magnitude to the global linear hydrophobic moment as the one or more additional residue centroids by mapping each residue at a same distance from a center of the protein structure;

use the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

output the global linear hydrophobic moment to a user.

15. (Original) The apparatus of claim 14, wherein the centroid of the residue centroids represents a geometric center of the tertiary protein structure.

16. (Cancelled)

17. (Original) The apparatus of claim 14, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

18. (Canceled)

19. (Original) The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.

20. (Original) The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

21. (Presently amended) An article of manufacture for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, comprising:

a computer-readable medium having computer-readable code embodied thereon, the computer-readable code comprising:

a step to calculate a centroid of residue centroids;

a step to use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

a step to calculate a first-order hydrophobic moment;

a step to enhance correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

a step to use the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to define the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, and wherein each residue centroid having a same fractional distance to a surface of the tertiary protein structure as one or more additional residue centroids contributes an equivalent magnitude to the global linear hydrophobic moment as the one or more additional residue centroids by mapping each residue at a same distance from a center of the protein structure;

a step to use the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

a step to output the global linear hydrophobic moment to a user.